

Phase Behavior of Polyampholytes from Charged Hard-Sphere Chain Model

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A molecular thermodynamic theory developed for polyelectrolytes (PEs) is extended for polyampholytes (PAs) on the basis of the coarse-grained charged hard-sphere chain model. Consistent with simulation results and experimental observations, the phase behavior of neutral PAs with variations in sequence and chain length is successfully predicted by the theory. At a fixed chain length, the phase envelope expands as the sequence of charge distribution becomes less random. With increasing chain length, the phase envelope expands for random and diblock PAs, but shrinks for zwitterionic PAs. The predicted critical temperature, density, and pressure show a nice scaling relationship with chain length for all the three (random, diblock, and zwitterionic) PAs.